

# On helicity and spin on the light cone

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Starting from a one-body front-form equation with Lepage-Brodsky spinors we show, with a fair amount of new technology, how an integral equation in standard momentum space with Björken-Drell spinors can be obtained. The integral equation decouples for singlets and triplets. HCP 20Oct/20 Nov 2001

## 1. Introduction

We address to Eq.(96) of [1],

$$M^2 \psi_{\lambda_1 \lambda_2}(x, \vec{k}_\perp) = \sum_{\lambda'_1, \lambda'_2} \int dx' d^2 \vec{k}'_\perp \times U_{\lambda_1 \lambda_2; \lambda'_1 \lambda'_2}(x, \vec{k}_\perp; x', \vec{k}'_\perp) \psi_{\lambda'_1 \lambda'_2}(x', \vec{k}'_\perp) + \left[ \frac{m_1^2 + \vec{k}_\perp^2}{x} + \frac{m_2^2 + \vec{k}_\perp^2}{1-x} \right] \psi_{\lambda_1 \lambda_2}(x, \vec{k}_\perp), \quad (1)$$

a one-body integral equation with the kernel

$$U_{\lambda_1 \lambda_2; \lambda'_1 \lambda'_2}(x, \vec{k}_\perp; x', \vec{k}'_\perp) = -\frac{4m_1 m_2}{3\pi^2} \times \frac{\bar{\alpha}(Q)}{Q^2} R(Q) \frac{S_{\lambda_1 \lambda_2; \lambda'_1 \lambda'_2}(x, \vec{k}_\perp; x', \vec{k}'_\perp)}{\sqrt{x(1-x)x'(1-x')}}, \quad (2)$$

and refer to [2] and [3] for more background information. Here,  $M^2$  is the wanted eigenvalue of the invariant mass squared operator, with associated eigenfunction  $\psi \equiv \Psi_{q\bar{q}}$ . It is the probability amplitude for finding in the  $q\bar{q}$ -space a quark with the effective (constituent) mass  $m_1$ , longitudinal momentum fraction  $x$ , transversal momentum  $\vec{k}_\perp$  and helicity  $\lambda_1$ , and correspondingly for the anti-quark with  $m_2$ ,  $1-x$ ,  $-\vec{k}_\perp$  and  $\lambda_2$ .

The spinor factor  $S_{\lambda_1 \lambda_2; \lambda'_1 \lambda'_2}$  is tabulated explicitly in [5]. It is defined in terms of Lepage-Brodsky spinors [4,5],

$$S_{\lambda_1 \lambda_2; \lambda'_1 \lambda'_2}(x, \vec{k}_\perp; x', \vec{k}'_\perp) = [\bar{u}(k_1, \lambda_1) \gamma^\mu u(k'_1, \lambda'_1)] [\bar{u}(k_2, \lambda_2) \gamma_\mu u(k'_2, \lambda'_2)]. \quad (3)$$

But contrary to [5], the  $u$ -spinors are normalized here:  $\bar{u}(k, \lambda) u(k, \lambda') = \delta_{\lambda\lambda'}$ . Due to the helicity

indices, the one-body equation in Eq.(1) is a set of four coupled integral equations in the three momentum components  $x$  and  $\vec{k}_\perp$ .

Our aim is to convert Eq.(1) into a set of integral equations in usual momentum space.

## 2. Helicity and spin

The Lepage-Brodsky spinors  $u(p, \lambda)$ , as tabulated in the appendix of Ref. [4], are:

$$u^{LB}(p, \lambda) = \frac{1}{\sqrt{4mp^+}} \begin{pmatrix} p^+ + m & -p_l \\ p_r & p^+ + m \\ p^+ - m & p_l \\ p_r & -p^+ + m \end{pmatrix} \quad (4)$$

for  $\lambda : \uparrow\downarrow$ , with  $p_r \equiv p_x + ip_y$  and  $p_l \equiv p_x - ip_y$ . They differ from the Björken-Drell spinors [7],

$$u^{BD}(p, s) = \frac{1}{\sqrt{2m(E+m)}} \begin{pmatrix} E+m & 0 \\ 0 & E+m \\ p_z & p_l \\ p_r & -p_z \end{pmatrix} \quad (5)$$

for  $s : \uparrow\downarrow$ , with  $E \equiv E(p) = \sqrt{m^2 + \vec{p}_\perp^2 + p_z^2}$ .

Both spinors are solutions to the same equation, the free Dirac equation  $(\not{p} - m)u(p, \lambda) = 0$  and are normalized in the same way. Hence, they must be linear superpositions of each other:

$$u_\alpha^{BD}(p, s) = \sum_\lambda u_\alpha^{LB}(p, \lambda) \omega_{\lambda s}. \quad (6)$$

The transformation matrix can be constructed easily by projection with the appropriate adjoint

spinor. We get

$$\omega_{\lambda s} = \sum_{\alpha} \bar{u}_{\alpha}^{LB}(p, \lambda) u_{\alpha}^{BD}(p, s). \quad (7)$$

Calculating the four overlap matrix elements explicitly with the corresponding spinors yields:

$$\omega_{\lambda s} = \begin{pmatrix} m + p^+ & p_l \\ -p_r & m + p^+ \end{pmatrix} \frac{1}{\sqrt{2p^+(E + m)}}, \quad (8)$$

with the rows labeled by the helicity  $\lambda = \uparrow \downarrow$  and the columns by the spin  $s = \uparrow \downarrow$ . This transformation is unitary. It is called a Melosh transformation [8–10]. The matrix  $\omega_{\lambda s}$  has dimension  $2 \times 2$  in our case (fermions). For higher spins these matrices are larger; they have dimension  $(2j + 1) \times (2j + 1)$ . The unitarity relation  $\omega \omega^\dagger = \omega^\dagger \omega = 1$  can be verified easily by

$$\sum_s \omega_{\lambda s} \omega_{s \lambda'}^* = \delta_{\lambda \lambda'} = \frac{1}{2p^+(E + m)} \times \begin{pmatrix} m + p^+ & p_l \\ -p_r & m + p^+ \end{pmatrix} \begin{pmatrix} m + p^+ & -p_l \\ p_r & m + p^+ \end{pmatrix}, \quad (9)$$

since  $(p^+ + m)^2 + p_l p_r = 2p^+(E + m)$ .

The spinors appear in bilinear combinations. It is therefore convenient to define the  $4 \times 4$  matrix

$$\Omega_{\lambda_1 \lambda_2; s_1 s_2} = \omega_{\lambda_1 s_1} \omega_{\lambda_2 s_2} \quad (10)$$

as the unitary direct product of the  $\omega$ 's. In consequence one can apply a unitary transformation to generate a new spinor factor

$$\tilde{S}_{s_1 s_2; s'_1 s'_2} = (\Omega^\dagger S \Omega)_{s_1 s_2; s'_1 s'_2} = [\bar{u}(k_1, s_1) \gamma^\mu u(k'_1, s'_1)] [\bar{u}(k_2, s_2) \gamma_\mu u(k'_2, s'_2)], \quad (11)$$

which looks like  $S$  except that Lepage–Brodsky are replaced by Björken–Drell spinors.

The BD–spinors of Eq.(5) transform under spatial rotations like a half-integer representation of the rotation group  $|t s\rangle$  with spin  $t = \frac{1}{2}$  and projection  $s = \pm \frac{1}{2}$  [11]. Two such spin states can be coupled to a state with total spin  $T = 0$  or  $T = 1$ . Particularly, the function

$$W_{TS} = \sum_{s_1, s_2} \langle t_1 s_1 t_2 s_2 | TS \rangle u(k_1, s_1) u(k_2, s_2),$$

with  $t_1 = t_2 = \frac{1}{2}$ , transforms like a function of  $k_1$  and  $k_2$  with total spin  $T$  and projection

$S = -T, -T + 1, \dots, T$ . The Clebsch–Gordan coefficients  $\langle t_1 s_1 t_2 s_2 | TS \rangle \equiv C_{s_1 s_2; TS}$  are real in the Condon–Shortley phase convention [11] and define an unitary transformation. We use it to define yet a third spinor factor  $\bar{S}$

$$\begin{aligned} \bar{S}_{TS; T' S'} &= (C^\dagger \tilde{S} C)_{TS; T' S'} \\ &= (C^\dagger \Omega^\dagger S \Omega C)_{TS; T' S'} \end{aligned} \quad (12)$$

and proceed.

### 3. Transforming the integral equation

In comparing Lepage–Brodsky and Björken–Drell spinors we have used tacitly the relation between the instant form  $p_z$  and the front form  $p^+ = p_z + \sqrt{m^2 + \vec{p}_\perp^2 + p_z^2}$ . This is correct, since the Dirac spinors are defined only for free particles. Dealing with two particles, and two spinors  $u(k_1, s_1)$  and  $u(k_2, s_2)$ , one can assume that they have opposite three-momenta  $\vec{k}_1 = -\vec{k}_2 = \vec{k}$ . Thus, their  $k^+$  and total  $K^+ = k_1^+ + k_2^+$  are related to  $k_z$  (with  $\vec{k} = (\vec{k}_\perp, k_z)$ ). One can introduce even a momentum fraction  $x = k_1^+/K^+$  and relate it to  $k_z$  by

$$x(k_z) = \frac{E_1 + k_z}{E_1 + E_2} \quad (13)$$

with  $E_{1,2} \equiv E_{1,2}(k) = \sqrt{m_{1,2}^2 + k_z^2 + \vec{k}_\perp^2}$ . But here is a subtle point: The so defined  $x$  is conceptually different from the longitudinal momentum fraction in Eq.(1) which is  $x = k_1^+/P^+$ . The  $P^+$  contains the interaction [4], the  $K^+$  does not.

However, there is one common aspect: While  $k_z$  varies from  $-\infty$  to  $+\infty$ , the  $x(k_z)$  in Eq.(13) varies from 0 to 1. It has thus the same domain of validity as the momentum fractions of Eq.(1). Eq.(13) can be used therefore to transform integration variables in Eq.(1) from  $(x, \vec{k}_\perp)$  to  $\vec{k}$ , such that all three components of  $\vec{k}$  have the same domain. In numerical work this is more than convenient. The transformation in Eq.(13) has thus been used tacitly in all past numerical work. New is here, that we use Eq.(13) explicitly to transform Eq.(1).

Transforming variables, the Jacobian is [5]

$$dx = \frac{x(1-x)}{A(k)} \frac{dk_z}{m_r}. \quad (14)$$

The reduced mass  $m_r$  takes care of the dimensions since  $A(k)$  is dimensionless,

$$\frac{1}{A(k)} = \frac{m_r}{E_r} = m_r \left( \frac{1}{E_1} + \frac{1}{E_2} \right). \quad (15)$$

The diagonal part of Eq.(1) becomes

$$\frac{m_1^2 + \vec{k}_\perp^2}{x} + \frac{m_2^2 + \vec{k}_\perp^2}{1-x} = (E_1(k) + E_2(k))^2. \quad (16)$$

Substituting all of that in Eq.(1) gives at first

$$\begin{aligned} M^2 \psi_{\lambda_1 \lambda_2}(\vec{k}) &= \sum_{\lambda'_1, \lambda'_2} \int \frac{d^3 \vec{k}'}{m_r} \frac{x'(1-x')}{A(k')} \\ &\quad \times U_{\lambda_1 \lambda_2; \lambda'_1 \lambda'_2}(\vec{k}; \vec{k}') \psi_{\lambda'_1 \lambda'_2}(\vec{k}') \\ &\quad + (E_1(k) + E_2(k))^2 \psi_{\lambda_1 \lambda_2}(\vec{k}). \end{aligned} \quad (17)$$

Due to the Jacobian, the effective kernel

$$\frac{x'(1-x')}{A(k')} U(\vec{k}; \vec{k}') \quad (18)$$

ceases to be symmetric in  $\vec{k}$  and  $\vec{k}'$ . The asymmetry, however, can be removed by introducing the reduced wave function  $\varphi_{s_1 s_2}(\vec{k})$  defined by

$$\begin{aligned} \psi_{\lambda_1 \lambda_2}(\vec{k}) &= \frac{\Phi_{\lambda_1 \lambda_2}(\vec{k})}{\sqrt{x(1-x)}}, \\ \Phi_{\lambda_1 \lambda_2}(\vec{k}) &= \sqrt{A(k)} \sum_{s_1, s_2} \Omega_{\lambda_1 \lambda_2; s_1 s_2} \varphi_{s_1 s_2}(\vec{k}). \end{aligned} \quad (19)$$

The equation for  $\varphi_{s_1 s_2}$  is then

$$\begin{aligned} &\left[ M^2 - (E_1(k) + E_2(k))^2 \right] \varphi_{s_1 s_2}(\vec{k}) \\ &= \sum_{s'_1, s'_2} \int d^3 \vec{k}' \tilde{U}_{s_1 s_2; s'_1 s'_2}(\vec{k}; \vec{k}') \varphi_{s'_1 s'_2}(\vec{k}'). \end{aligned} \quad (20)$$

The kernel, with  $m_s = m_1 + m_2$ , is

$$\tilde{U}_{s_1 s_2; s'_1 s'_2} = -\frac{4m_s}{3\pi^2} \frac{\bar{\alpha}(Q)}{Q^2} R(Q) \frac{\tilde{S}_{s_1 s_2; s'_1 s'_2}}{\sqrt{A(k)A(k')}}, \quad (21)$$

with the BD spinor factor  $\tilde{S}$  given in Eq.(11).

#### 4. Doing even better

The asymmetry can also be removed by introducing another reduced wave function  $\bar{\varphi}_{TS}(\vec{k})$ , *i.e.* replacing the  $\Phi$  in Eq.(19) by

$$\Phi_{\lambda_1 \lambda_2}(\vec{k}) = \sqrt{A(k)} \sum_{T, S} (\Omega C)_{\lambda_1 \lambda_2; TS} \bar{\varphi}_{TS}(\vec{k}). \quad (22)$$

The equation for  $\bar{\varphi}_{TS}$  becomes then

$$\begin{aligned} &\left[ M^2 - (E_1(k) + E_2(k))^2 \right] \bar{\varphi}_{TS}(\vec{k}) \\ &= \sum_{T', S'} \int d^3 \vec{k}' \bar{U}_{TS; T' S'}(\vec{k}; \vec{k}') \bar{\varphi}_{T' S'}(\vec{k}'), \end{aligned} \quad (23)$$

with the kernel ( $m_s = m_1 + m_2$ )

$$\bar{U}_{TS; T' S'} = -\frac{4m_s}{3\pi^2} \frac{\bar{\alpha}(Q)}{Q^2} R(Q) \frac{\bar{S}_{TS; T' S'}}{\sqrt{A(k)A(k')}}. \quad (24)$$

Since  $\bar{U}_{TS; T' S'}$  is block diagonal, as shown in the appendix, one can divide the set of 4 equations into an uncoupled equation for the singlets

$$\begin{aligned} &\left[ M^2 - (E_1(k) + E_2(k))^2 \right] \bar{\varphi}_{00}(\vec{k}) \\ &= \int d^3 \vec{k}' \bar{U}_{00}(\vec{k}; \vec{k}') \bar{\varphi}_{00}(\vec{k}'), \end{aligned} \quad (25)$$

and a set of 3 coupled equations for the triplets. They look like Eq.(24) except that the sum over  $T = T' = 1$  is absent. The singlet kernel is

$$\bar{U}_{00} = -\frac{4m_s}{3\pi^2} \frac{\bar{\alpha}(Q)}{Q^2} R(Q) \frac{\bar{S}_{00}}{\sqrt{A(k)A(k')}}, \quad (26)$$

with singlet spinor function given in Eq.(50). For equal masses  $m_1 = m_2$ , it reduces to

$$\bar{S}_{00} = \bar{N} [1 + 3\vec{k}^2 + 3\vec{k}'^2 + \vec{k}^2 \vec{k}'^2 - (\vec{k} \vec{k}')(\vec{k} \vec{k}')], \quad (27)$$

with the famous hyperfine coefficient 3. One can thus calculate eigenvalues and eigenfunctions for the singlets separately from those of the triplets!

It is possible to simplify the triplet equations even further, by coupling (in the spinor function) the total spin  $\vec{T}$  with the (intrinsic) orbital angular momentum  $\vec{\ell}$  to good total momentum  $\vec{J} = \vec{\ell} + \vec{T}$ , but this exceeds the limitations of these proceedings, and will be given elsewhere.

#### 5. Conclusion

We seem to have got the cookie and the cake.

#### 6. Acknowledgements

AK was supported by the Max-Planck Institut für Kernphysik, Heidelberg, by EU contract

number HPCF-CT-2001-00385 with the European Commission High-Level Scientific Conferences for the workshop TRENTO 2001 as a young researcher, and by Austrian FWF research grant Nr. P14794.- HCP thanks with pleasure Tobias Frederico from Sao Paulo for verifying independently some of the results.

## A. Spinors and currents

The Björken-Drell spinor  $u$  is

$$u(p, s) = \sqrt{\frac{E+m}{2m}} \begin{pmatrix} \vec{\sigma} \cdot \vec{p} & \chi_s \\ E+m & \chi_s \end{pmatrix}, \quad (28)$$

with the Pauli spinors  $\chi_{\uparrow\downarrow}$ . In compact notation

$$\vec{k}_1 = \frac{\vec{p}}{E_1 + m_1}, \quad \vec{k}_2 = \frac{\vec{p}}{E_2 + m_2}, \quad (29)$$

$$N_1 = \sqrt{\frac{E_1 + m_1}{2m_1}}, \quad N_2 = \sqrt{\frac{E_2 + m_2}{2m_2}},$$

the spinors become for  $\vec{p}_1 = -\vec{p}_2 = \vec{p}$

$$u(p_1, s_1) = N_1 \begin{pmatrix} \chi_{s_1} \\ \vec{\sigma} \cdot \vec{k}_1 \chi_{s_1} \end{pmatrix}, \quad (30)$$

$$u(p_2, s_2) = N_2 \begin{pmatrix} \chi_{s_2} \\ -\vec{\sigma} \cdot \vec{k}_2 \chi_{s_2} \end{pmatrix}.$$

The time-component of the current becomes

$$[\bar{u}(p, s) \gamma^0 u(p', s')] = NN' \langle s | 1 + (\vec{\sigma} \cdot \vec{k})(\vec{\sigma} \cdot \vec{k}') | s' \rangle. \quad (31)$$

Since  $(\vec{\sigma} \cdot \vec{k})(\vec{\sigma} \cdot \vec{k}') = \vec{k} \cdot \vec{k}' + i\vec{\sigma} \cdot (\vec{k} \wedge \vec{k}')$  we abbreviate

$$K = 1 + \vec{k} \cdot \vec{k}', \quad \vec{R} = i(\vec{k} \wedge \vec{k}'), \quad (32)$$

to get in compact notation

$$[\bar{u}(p, s) \gamma^0 u(p', s')] = NN' \langle s | K + \vec{\sigma} \cdot \vec{R} | s' \rangle \\ = NN' \begin{pmatrix} K + \vec{e}_z \cdot \vec{R} & \vec{e}_l \cdot \vec{R} \\ \vec{e}_r \cdot \vec{R} & -K - \vec{e}_z \cdot \vec{R} \end{pmatrix}, \quad (33)$$

with  $\vec{e}_l \equiv \vec{e}_x - i\vec{e}_y$  and  $\vec{e}_r \equiv \vec{e}_x + i\vec{e}_y$  and the unit vectors in the three space directions  $\vec{e}_x, \vec{e}_y, \vec{e}_z$ . The space-component of the current becomes

$$[\bar{u}(p, s) \vec{\gamma} u(p', s')] = NN' \langle s | (\vec{\sigma} \cdot \vec{k})\vec{\sigma} + \vec{\sigma}(\vec{\sigma} \cdot \vec{k}') | s' \rangle. \quad (34)$$

With  $(\vec{k} \cdot \vec{\sigma})\vec{\sigma} = \vec{k} + i(\vec{\sigma} \wedge \vec{k})$  and correspondingly with  $\vec{\sigma}(\vec{k}' \cdot \vec{\sigma}) = \vec{k}' - i(\vec{\sigma} \wedge \vec{k}')$ , we abbreviate

$$\vec{S} = \vec{k} + \vec{k}', \quad \vec{D} = i(\vec{k} - \vec{k}') \quad , \quad (35)$$

to get in compact notation

$$[\bar{u}(p, s) \vec{\gamma} u(p', s')] = NN' \langle s | \vec{S} + \vec{\sigma} \wedge \vec{D} | s' \rangle \\ = NN' \begin{pmatrix} \vec{S} + \vec{e}_z \wedge \vec{D} & \vec{e}_l \wedge \vec{D} \\ \vec{e}_r \wedge \vec{D} & -\vec{S} - \vec{e}_z \wedge \vec{D} \end{pmatrix}. \quad (36)$$

It helps to evaluate the matrix elements of  $\tilde{S}$ .

## B. The spinor factor $\tilde{S}$

We want to calculate the spinor factor

$$\tilde{S}_{s_1 s_2; s'_1 s'_2}(\vec{p}; \vec{p}') \\ = [\bar{u}(p_1, s_1) \gamma^\mu u(p'_1, s'_1)] [\bar{u}(p_2, s_2) \gamma_\mu u(p'_2, s'_2)] \\ = [\bar{u}(p_1, s_1) \gamma^0 u(p'_1, s'_1)] [\bar{u}(p_2, s_2) \gamma^0 u(p'_2, s'_2)] \\ - [\bar{u}(p_1, s_1) \vec{\gamma} u(p'_1, s'_1)] [\bar{u}(p_2, s_2) \vec{\gamma} u(p'_2, s'_2)] \quad (37)$$

and arrange it for this purpose as the matrix

$$\begin{bmatrix} \tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} & \tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} & \tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} & \tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} \\ \tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} & \tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} & \tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} & \tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} \\ \tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} & \tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} & \tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} & \tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} \\ \tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} & \tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} & \tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} & \tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} \end{bmatrix} = \begin{bmatrix} \tilde{S}_{11} & \tilde{S}_{21} & \tilde{S}_{31} & \tilde{S}_{41} \\ \tilde{S}_{12} & \tilde{S}_{22} & \tilde{S}_{32} & \tilde{S}_{42} \\ \tilde{S}_{13} & \tilde{S}_{23} & \tilde{S}_{33} & \tilde{S}_{43} \\ \tilde{S}_{14} & \tilde{S}_{24} & \tilde{S}_{34} & \tilde{S}_{44} \end{bmatrix}. \quad (38)$$

Its elements become with the above abbreviations

$$\tilde{S}_{s_1 s_2; s'_1 s'_2}(\vec{p}; \vec{p}') \\ = \bar{N} \langle s_1 | K + \vec{\sigma} \cdot \vec{R} | s'_1 \rangle \langle s_2 | K + \vec{\sigma} \cdot \vec{R} | s'_2 \rangle \\ + \bar{N} \langle s_1 | \vec{S} + \vec{\sigma} \wedge \vec{D} | s'_1 \rangle \langle s_2 | \vec{S} + \vec{\sigma} \wedge \vec{D} | s'_2 \rangle, \quad (39)$$

where  $\bar{N} \equiv N_1 N'_1 N_2 N'_2$ . Prior to explicit calculation, we mention the obvious symmetries of Eq.(37), namely (1) hermiticity, and (2) symmetry under the particle exchange  $1 \leftrightarrow 2$ . Since the momenta are back to back, one can restrict to  $s_1, s_2 \leftrightarrow s_2, s_1$ , to spin exchange, which generates the symmetries:  $\tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} = \tilde{S}_{\downarrow\uparrow; \downarrow\uparrow}$ ,  $\tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} = \tilde{S}_{\downarrow\uparrow; \uparrow\downarrow}$ ,  $\tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} = \tilde{S}_{\downarrow\uparrow; \uparrow\downarrow}$ , and  $\tilde{S}_{\uparrow\downarrow; \uparrow\downarrow} = \tilde{S}_{\downarrow\uparrow; \uparrow\downarrow}$ . Together with  $\tilde{S}_{\uparrow\uparrow; \uparrow\uparrow} = \tilde{S}_{\downarrow\downarrow; \downarrow\downarrow}$ , one has the five relations

$$\tilde{S}_{11} = \tilde{S}_{22}; \quad \tilde{S}_{12} = \tilde{S}_{21}; \\ \tilde{S}_{13} = \tilde{S}_{23}; \quad \tilde{S}_{14} = \tilde{S}_{24}; \quad \tilde{S}_{44} = \tilde{S}_{33}. \quad (40)$$

The real non-trivial matrix elements become:

$$\tilde{S}_{11} = K_1 K_2 + \vec{S}_1 \vec{S}_2 - \vec{D}_1 \vec{D}_2 - R_{1z} R_{2z} + D_{1z} D_{2z} \\ \tilde{S}_{12} = \vec{R}_1 \vec{R}_2 + \vec{D}_1 \vec{D}_2 - R_{1z} R_{2z} + D_{1z} D_{2z} \\ \tilde{S}_{33} = K_1 K_2 + \vec{S}_1 \vec{S}_2 + \vec{D}_1 \vec{D}_2 + R_{1z} R_{2z} - D_{1z} D_{2z}. \quad (41)$$

The overall factor  $\overline{N}$  is omitted here to fit the expressions in one line. The non-trivial off-diagonal matrix elements are the complex functions:

$$\begin{aligned}\tilde{S}_{13} &= (K_1 + R_{1z})R_{1r} - D_{1z}D_{2r} - (\vec{S}_1 \wedge \vec{D}_2)_z \\ \tilde{S}_{14} &= (K_1 - R_{1z})R_{2l} - D_{1z}D_{2r} - (\vec{S}_1 \wedge \vec{D}_2)_l \\ \tilde{S}_{34} &= R_{1l}R_{2l} - D_{1l}D_{2l},\end{aligned}\quad (42)$$

where for example  $R_{1r} = \vec{e}_r \cdot \vec{R}_1$ . — We like to demonstrate the calculation at hand of two examples. One begins with inserting the spin projections into Eq.(37). For  $S_{12} = \tilde{S}_{\uparrow\downarrow;\uparrow\uparrow}$  one has

$$\begin{aligned}\tilde{S}_{12} &= \overline{N} \langle \uparrow | K_1 + \vec{\sigma} \cdot \vec{R}_1 | \downarrow \rangle \langle \downarrow | K_2 + \vec{\sigma} \cdot \vec{R}_2 | \uparrow \rangle \\ &+ \overline{N} \langle \uparrow | \vec{S}_1 + \vec{\sigma} \wedge \vec{D}_1 | \downarrow \rangle \langle \downarrow | \vec{S}_2 + \vec{\sigma} \wedge \vec{D}_2 | \uparrow \rangle.\end{aligned}\quad (43)$$

Inserting Eqs. (33) and (36) gives

$$\begin{aligned}\tilde{S}_{12} &= \overline{N} [ (\vec{e}_r \cdot \vec{R}_1)(\vec{e}_l \cdot \vec{R}_2) + (\vec{e}_r \wedge \vec{D}_1)(\vec{e}_l \wedge \vec{D}_2) ] \\ &= \overline{N} [ (\vec{e}_x \cdot \vec{R}_1)(\vec{e}_x \cdot \vec{R}_2) + (\vec{e}_y \cdot \vec{R}_1)(\vec{e}_y \cdot \vec{R}_2) \\ &+ (\vec{e}_x \wedge \vec{D}_1)(\vec{e}_x \wedge \vec{D}_2) + (\vec{e}_y \wedge \vec{D}_1)(\vec{e}_y \wedge \vec{D}_2) ].\end{aligned}\quad (44)$$

From the vector identity

$$(\vec{A} \wedge \vec{B}) \cdot (\vec{C} \wedge \vec{D}) = (\vec{A} \cdot \vec{C})(\vec{B} \cdot \vec{D}) - (\vec{A} \cdot \vec{D})(\vec{B} \cdot \vec{C}) \quad (45)$$

follows most directly Eq.(41). — Continuing with  $\tilde{S}_{11} = S_{\uparrow\downarrow;\uparrow\downarrow}$ , we skip the first step and get:

$$\begin{aligned}\tilde{S}_{11} &= \overline{N} [ (K_1 + \vec{e}_z \cdot \vec{R}_1)(K_2 - \vec{e}_z \cdot \vec{R}_2) \\ &+ (\vec{S}_1 + \vec{e}_z \wedge \vec{D}_1)(\vec{S}_2 - \vec{e}_z \wedge \vec{D}_2) ].\end{aligned}\quad (46)$$

Applying Eq.(45) gives directly Eq.(41).

### C. The spinor factor $\overline{S}$

Transforming unitarily to  $\overline{S} = C^\dagger \tilde{S} C$ , taking the Clebsch-Gordan coefficients from Table 5.2 of [11], i.e.  $C_{s_1 s_2; TS} \equiv \langle t_1 s_1 t_2 s_2 | TS \rangle$ :

$$C_{s_1 s_2; TS} = \begin{bmatrix} & 00 & 10 & 1+1 & 1-1 \\ \uparrow\downarrow & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ \downarrow\uparrow & \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ \uparrow\uparrow & 0 & 0 & 1 & 0 \\ \downarrow\downarrow & 0 & 0 & 0 & 1 \end{bmatrix}, \quad (47)$$

and carrying out the matrix product, gives

$$\overline{S} = \begin{bmatrix} \tilde{S}_{11} - \tilde{S}_{12} & 0 & 0 & 0 \\ 0 & \tilde{S}_{22} + \tilde{S}_{12} & \sqrt{2} \tilde{S}_{31} & \sqrt{2} \tilde{S}_{41} \\ 0 & \sqrt{2} \tilde{S}_{13} & \tilde{S}_{33} & \tilde{S}_{43} \\ 0 & \sqrt{2} \tilde{S}_{14} & \tilde{S}_{34} & \tilde{S}_{44} \end{bmatrix}. \quad (48)$$

One needs only the symmetry relations in Eq.(40) to derive this result. Denoting the diagonal elements by  $\overline{S}_{TS}$ , one has thus  $\overline{S}_{00} = \tilde{S}_{11} - \tilde{S}_{12}$  and  $\overline{S}_{10} = \tilde{S}_{22} + \tilde{S}_{12}$ , or explicitly from Eq.(41)

$$\begin{aligned}\overline{S}_{00} &= \overline{N} [ K_1 K_2 + \vec{S}_1 \cdot \vec{S}_2 - \vec{R}_1 \cdot \vec{R}_2 - 2 \vec{D}_1 \cdot \vec{D}_2 ] \\ \overline{S}_{10} &= \overline{N} [ K_1 K_2 + \vec{S}_1 \cdot \vec{S}_2 + \vec{R}_1 \cdot \vec{R}_2 - 2 R_{1z} R_{2z} \\ &+ 2 D_{1z} D_{2z} ].\end{aligned}\quad (49)$$

By inspection, the singlet matrix element  $S_{00}$  is a rotational scalar. To get it explicitly, the abbreviations in Eqs.(32) and (35) are restored:

$$\begin{aligned}\overline{S}_{00} &= \overline{N} [ (1 + \vec{k}_1 \cdot \vec{k}'_1)(1 + \vec{k}_2 \cdot \vec{k}'_2) + (\vec{k}_1 \wedge \vec{k}'_1)(\vec{k}_2 \wedge \vec{k}'_2) \\ &+ (\vec{k}_1 + \vec{k}'_1)(\vec{k}_2 + \vec{k}'_2) + 2(\vec{k}_1 - \vec{k}'_1)(\vec{k}_2 - \vec{k}'_2) ]\end{aligned}$$

or after evaluating the wedge products

$$\begin{aligned}\overline{S}_{00} &= \overline{N} [ 1 + 3\vec{k}_1 \cdot \vec{k}_2 + 3\vec{k}'_1 \cdot \vec{k}'_2 + (\vec{k}_1 \cdot \vec{k}_2)(\vec{k}'_1 \cdot \vec{k}'_2) \\ &- (\vec{k}_1 \cdot \vec{k}'_2)^2 + (\vec{k}_1 - \vec{k}_2)(\vec{k}'_1 - \vec{k}'_2) ].\end{aligned}\quad (50)$$

For equal masses, with  $\vec{k}_1 = \vec{k}_2$ , this reduces to Eq.(27). On remains with the problem to diagonalize  $\overline{S}$  in the triplet space.

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